THEOCHEM, VOLUME 56 (1989)

(*Journal of Molecular Structure, Vol. 187*)

AUTHOR INDEX

Alagona, G., 219
Angelov, S., 23
Atanasov, M., 23
Avbelj, F., 307

Bertrán, J., 55
Bock, Ch.W., 69
Bolotin, A., 291
Bourasseau, S., 251
Buemi, G., 325

Coitiño, E.L., 55
Cyvin, S.J., 285

Danovich, D., 297
De Ranter, C.J., 161
Dewar, M.J.S., 1
Domnina, E., 297

Epiotis, N.D., 359
Ewbank, J.D., 271

Fabian, W.M.F., 199
Flakus, H.T., 35

Gandolfo, C., 325
Ghio, C., 219
Gopinathan, M.S., 169
Gutman, I., 285

Hadži, D., 307
Hagler, A.T., 123
Henriet, Ch., 233
Honegger, E., 261

Imoto, M., 317
Ishii, M., 209

Jie, C., 1

Karpas, Z., 123
Kibler, M., 83
Kikuchi, O., 209
Kollenz, G., 199

Leroy, G., 233, 251
Lledós, A., 55
Lowrey, A.H., 177

Marsden, C.J., 337
Mavri, J., 307
Mayer, I., 23
Mitchell, T.J., 115
Morihashi, K., 209
Murray, J.S., 95

Nagy, P., 219
Naumov, V.A., 191

Panchenko, Yu.N., 69
Peeters, D., 251
Pipiraite, P., 291
Politzer, P., 95

Ružiene, A., 291

Sakai, S., 317
Sana, M., 233, 251
Schafer, L., 271
Schulz, L., 15
Seminario, J.M., 95
Sheng, R.-Q., 285
Siam, K., 271
Siddarth, P., 169
Smith, B.J., 337
Stern, P.S., 123
Sussman, F., 123

Tute, M.S., 115

Van Alsenoy, C., 271
Van Hooydonk, G., 109
Ventura, O.N., 55
Verlinde, C.L., 161
Von Szentpály, L., 139

Webb, G.A., 115
Wilante, C., 251

Zakrzewski, V., 297
Zuev, M.B., 191

THEOCHEM, VOLUME 56 (1989)

(Journal of Molecular Structure, Vol. 187)

SUBJECT INDEX

N-Acetyl-L-pro-D-ala-*N'*-methyl tripeptide
Conformation of *N*-acetyl-L-pro-D-ala-*N'*-methyl tripeptide: empirical, semi-empirical MO and ab initio MO calculations, 307
Adrenergic activity
A theoretical study of the influence of noradrenaline ring fluorination on its adrenergic activity, 115
AM1
AM1 outer valence Green's function ionization energies of the azoles, 297
AM1 parameters
AM1 parameters for phosphorus, 1
AM1 study
AM1 study of hydrogen bonded complexes of water, 55
Amine
Theoretical investigation of the hindered amine photostabilising mechanism, 291
Angular dependence
Modelling of angular dependence of superexchange: application to copper(II) dimers, 23
Azines
A computational study of the structures and electrostatic potentials of some azines and nitroazines, 95
Azoles
AM1 outer valence Green's function ionization energies of the azoles, 297

B_2H_n
Theoretical study of B_2H_n (with $n=2$ to 6): molecules and related positive ions, 233
Benzenoid hydrocarbons
Remarks on Kekuléan and non-Kekuléan benzenoid hydrocarbons, 285
1,3-Butadiene
An ab initio structural investigation of 1,3-butadiene, isoprene and 2,3-dimethyl-1,3-butadiene rotamers, 69

Categories
Categories in chemistry and chemical computers, 15
CH_3SiF_3
Ab initio study of the structures and vibrational frequencies of CH_3SiF_3, $[CH_3SiF_4]^-$ and $[CH_3SiF_5]^{2-}$, 317
$[CH_3SiF_4]^-$
Ab initio study of the structures and vibrational frequencies of CH_3SiF_3, $[CH_3SiF_4]^-$ and $[CH_3SiF_5]^{2-}$, 317
$[CH_3SiF_5]^{2-}$
Ab initio study of the structures and vibrational frequencies of CH_3SiF_3, $[CH_3SiF_4]^-$ and $[CH_3SiF_5]^{2-}$, 317
Computers
Categories in chemistry and chemical computers, 15
Cooper pairs
On the absence of isotope effects in high-T_c superconductors and the role of (Cooper) pairs in bonding, 109
Copper(II) dimers
Modelling of angular dependence of superexchange: application to copper(II) dimers, 23
Crystal structures
Furan revisited: when to avoid ab initio studies on crystal structures, 161
Cycloaddition reactions
Novel [4+2] cycloaddition reactions of ketenimines: a semiempirical molecular orbital study, 199

Dimeric systems
On the vibrational transition selection rules for the centrosymmetric hydrogen-bonded dimeric systems, 35
Dimers
On the interconnection of metal–metal bonding in dimers and solid resistivity,

magnetic susceptibility, and normal superconductivity, 359
2,3-Dimethyl-1,3-butadiene
An ab initio structural investigation of 1,3-butadiene, isoprene and 2,3-dimethyl-1,3-butadiene rotamers, 69
Dithiin
Conformations and electronic structure of dithiin, 1,4-dithiino[2,3-*C*; 6,5-*C*′] diisothiazole and its derivatives, 325
Dithiino[2,3-*C*; 6,5-*C*′]diisothiazole
Conformations and electronic structure of dithiin, 1,4-dithiino[2,3-*C*; 6,5-*C*′] diisothiazole and its derivatives, 325

Electron density
On the relation between electron density, molecular structure and intramolecular forces in neutral and protonated formaldehyde and halogen substituted analogs, 123
Electrostatic potentials
A computational study of the structures and electrostatic potentials of some azines and nitroazines, 95
Ethane
The effect of geometrical relaxation on the rotational barrier of ethane, 261

F-omega model
Free electron PMO: *F*-omega model with variable electronegativity and self-interaction correction: application to ionic reaction intermediates, 139
Finite perturbation theory
Calculation of **g**-values of free radicals by finite perturbation theory, 209
Fluorination
A theoretical study of the influence of noradrenaline ring fluorination on its adrenergic activity, 115
Force constants
Ab initio force constants: a cautionary tale concerning nitrogen oxides, 337
Formaldehyde
On the relation between electron density, molecular structure and intramolecular forces in neutral and protonated formaldehyde and halogen substituted analogs, 123
Free electron PMO
Free electron PMO: *F*-omega model with variable electronegativity and self-interaction correction: application to ionic reaction intermediates, 139
Free radicals
Calculation of **g**-values of free radicals by finite perturbation theory, 209
Furan
Furan revisited: when to avoid ab initio studies on crystal structures, 161

g-values
Calculation of **g**-values of free radicals by finite perturbation theory, 209
Geometrical relaxation
The effect of geometrical relaxation on the rotational barrier of ethane, 261
Glyoxylic acid
Ab initio studies of structural features not easily amenable to experiment. Part 65. Ab initio molecular structures of glyoxylic, pyruvic, and propiolic acid, and comparison with microwave data, 271
Green's function ionization energies
AM1 outer valence Green's function ionization energies of the azoles, 297

Heats of formation
Heats of formation of some energetic compounds containing NO_2 and/or NF_2 groups, 251
Heterocycles
Strain in heterocycles, 169
High-T_c superconductors
On the absence of isotope effects in high-T_c superconductors and the role of (Cooper) pairs in bonding, 109
Hydrogen bonded complexes
AM1 study of hydrogen bonded complexes of water, 55
Hydrogen-bonded dimeric systems
On the vibrational transition selection rules for the centrosymmetric hydrogen-bonded dimeric systems, 35

Internal rotation
Ab initio study of internal rotation of the vinylphosphine molecule: $H_2C{=}CH{-}PH_2$, 191
Intramolecular forces
On the relation between electron density,

molecular structure and intramolecular forces in neutral and protonated formaldehyde and halogen substituted analogs, 123
Ionization energies
AM1 outer valence Green's function ionization energies of the azoles, 297
Isoprene
An ab initio structural investigation of 1,3-butadiene, isoprene and 2,3-dimethyl-1,3-butadiene rotamers, 69
Isotope effects
On the absence of isotope effects in high-T_c superconductors and the role of (Cooper) pairs in bonding, 109

Ketenimines
Novel [4+2] cycloaddition reactions of ketenimines: a semiempirical molecular orbital study, 199

Magnetic susceptibility
On the interconnection of metal–metal bonding in dimers and solid resistivity, magnetic susceptibility, and normal superconductivity, 359
Metal–metal bonding
On the interconnection of metal–metal bonding in dimers and solid resistivity, magnetic susceptibility, and normal superconductivity, 359
Molecular structure
On the relation between electron density, molecular structure and intramolecular forces in neutral and protonated formaldehyde and halogen substituted analogs, 123

N-aromatics
Theoretical calculations on the 1:1 complexes of N-aromatics with water, 219
NF_2
Heats of formation of some energetic compounds containing NO_2 and/or NF_2 groups, 251
Nitroazines
A computational study of the structures and electrostatic potentials of some azines and nitroazines, 95
Nitrogen oxides
Ab initio force constants: a cautionary tale concerning nitrogen oxides, 337
NO_2
Heats of formation of some energetic compounds containing NO_2 and/or NF_2 groups, 251
Noradrenaline ring
A theoretical study of the influence of noradrenaline ring fluorination on its adrenergic activity, 115

Periodic system of chemical elements
The periodic system of chemical elements: old and new developments, 83
Phosphorus
AM1 parameters for phosphorus, 1
Photostabilising mechanism
Theoretical investigation of the hindered amine photostabilising mechanism, 291
Propiolic acid
Ab initio studies of structural features not easily amenable to experiment. Part 65. Ab initio molecular structures of glyoxylic, pyruvic, and propiolic acid, and comparison with microwave data, 271
Pyruvic acid
Ab initio studies of structural features not easily amenable to experiment. Part 65. Ab initio molecular structures of glyoxylic, pyruvic, and propiolic acid, and comparison with microwave data, 271

Resistivity
On the interconnection of metal–metal bonding in dimers and solid resistivity, magnetic susceptibility, and normal superconductivity, 359
Rotational barrier
The effect of geometrical relaxation on the rotational barrier of ethane, 261

Strain
Strain in heterocycles, 169
Superconductivity
On the interconnection of metal–metal bonding in dimers and solid resistivity, magnetic susceptibility, and normal superconductivity, 359
Superexchange
Modelling of angular dependence of superexchange: application to copper(II) dimers, 23
Symmetric rotor models
Ab initio investigations of symmetric ro-

tor models for small trifluoromethyl substituted molecules, 177

Trifluoromethyl substituted molecules
Ab initio investigations of symmetric rotor models for small trifluoromethyl substituted molecules, 177

Vibrational transition selection
On the vibrational transition selection rules for the centrosymmetric hydrogen-bonded dimeric systems, 35

Vinylphosphine
Ab initio study of internal rotation of the vinylphosphine molecule: $H_2C=CH-PH_2$, 191

Water
AM1 study of hydrogen bonded complexes of water, 55
Theoretical calculations on the 1:1 complexes of N-aromatics with water, 219